Sampling versus filtering in Large-Eddy simulations

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A LES formalism in which the filter operator is replaced by a sampling operator is proposed. The unknown quantities that appear in the LES equations originate only from inadequate resolution (discretization errors). The resulting viewpoint seems to make a link between finite difference approaches and finite element methods. Sampling operators are shown to commute with nonlinearities and to be purely projective. Moreover, their use allows an unambiguous definition of the LES numerical grid. The price to pay is that sampling never commutes with spatial derivatives and the commutation errors must be modelled. It is shown that models for the discretization errors may be treated using the dynamic procedure. Preliminary results, using the Smagorinsky model, are very encouraging.

1. Introduction

The analysis presented here owes its origin to the unique practical motivation for Large-Eddy Simulations (LES's), i.e. the lack of adequate computational power. Indeed, LES is a discretization of the Navier-Stokes equations on a grid which is too coarse. Traditionally, the LES equations are presented as a smoothed version of the Navier-Stokes equations. The smoothing operation generates an unknown term that must be modelled. The solution of the LES equations also requires numerical schemes with, unavoidably, discretization errors. Since resolution is always the driving constraint in LES, the discretization errors are expected to play a significative role (Ghosal 1996; Kravchenko & Moin 1997; Chow & Moin 2003). However, several attempts have been proposed in order to minimize their effect on the large scale dynamics (Vasilyev *et al.* 1998; Marsden *et al.* 2002).

The viewpoint adopted in the approach developed here is very different, to such an extent that it might be viewed as provocative. This is however not the objective. The strategy that has been investigated is to abandon the idea of using smoothing filters. In that case, the discretization errors become the only term that requires a modelling effort. This viewpoint should not be confused with the MILES (Monotone Integrated Large Eddy Simulation) approach (Park *et al.* 2004) in which the numerical errors are expected to dissipate the correct amount of energy and to stabilize the under-resolved simulation. On the contrary, in the following, a real modelling effort is developed in order to account for the discretization errors. In particular, using the successful dynamic procedure, two embedded grids are used to optimize the model for the discretization errors.

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In spectral codes, filtering or reducing the resolution are two indistinguishable operations. In that sense, for these codes, the discretization errors and the modelling errors are identical and the methodology developed in this report would reduce to a simple re-interpretation of the LES equations without any practical consequence. For finite difference codes the situation is different. The filter width Δ_f and the grid spacing Δ_g may be considered as two independent parameters. In the limit $\Delta_g/\Delta_f \to 0$, the discretization errors are supposed to be negligible with respect to the "sub-filter" term. Due to finite computational ressources, such a limit is however never used in practice. A reasonable compromise is to consider that $\Delta_g/\Delta_f \lesssim 1$. In the following, the opposite limit ($\Delta_g/\Delta_f \to \infty$), obtained when no smoothing filter is used, is investigated for finite difference schemes. A bridge between the this approach and the traditional viewpoint is also proposed. The discretization scheme is considered to result from a sampling operation that shares some properties with filters.

2. Definitions

The purpose of this section is to introduce the sampling operators and to make the link between two apparently incompatible viewpoints on LES. The first one is the traditional filtering approach in which the Navier-Stokes velocity field u_i is transformed into a continuous filtered velocity $\tilde{u}_i$. The second viewpoint is the discrete representation $\overline{u}_i$ of the velocity field on a numerical grid in the actual LES simulation. In the filtering approach, the LES velocity $\tilde{u}_i$ is given by the following expression

$$\tilde{u}_i(\vec{x}) = \int G(\vec{x},\vec{y})\; u_i(\vec{y})\; d^3y\,, \tag{2.1}$$

in which, $G(\vec{x},\vec{y})$ is the filter kernel. In general, the filtered field depends on values of the original velocity field from the entire integration domain $\Omega \subset \mathbb{R}^3$. Very few constraints are imposed on the filter kernel $G(\vec{x},\vec{y})$ except that $G(\vec{x},\vec{y}) = 0$ for $\vec{y} \notin \Omega$ and the normalization condition:

$$\int G(\vec{x},\vec{y})\; d^3y = 1\,. \tag{2.2}$$

When considering the discrete representation of the signal u_i on the LES grid, the sampled signal is not a function from Ω into $\mathbb{R}$ anymore, but a mapping from the set of grid points $\{\vec{x}^\ell\}$ into $\mathbb{R}$. It is however possible to keep the same type of expression,

$$\overline{u}_i(\vec{x}) = \int H(\vec{x},\vec{y})\; u_i(\vec{y})\; d^3y\,. \tag{2.3}$$

In order to make the link with sampling and finite difference schemes, the discrete-filtered function $\overline{u}_i(\vec{x})$ should depend only on the grid values of $u_i(\vec{y})$, so that the general form of the kernel H has to be:

$$H(\vec{x},\vec{y}) = \sum_\ell h^\ell(\vec{x})\; \delta(\vec{y}-\vec{x}^\ell)\,, \tag{2.4}$$

and the discrete-filtered signal is given by:

$$\overline{u}_i(\vec{x}) = \sum_\ell h^\ell(\vec{x})\; u_i(\vec{x}^\ell)\,. \tag{2.5}$$

Such an expression amounts to assuming an interpolation of the signal between the grid points. However, only the values of the Navier-Stokes velocity on the grid are required to construct $\overline{u}_i$. Imposing a normalization condition on the discrete-filtering operator is also desirable. Since only the grid point values of $\overline{u}_i$ matter, it is sufficient to impose the normalization condition on the grid:

$$\int H(\vec{x}^{\ell_1},\vec{y})\; d^3y \;=\sum_{\ell_2}\; H^{\ell_1\ell_2} = 1\,, \tag{2.6}$$

where the square matrix $H^{\ell_1\ell_2} = h^{\ell_2}(\vec{x}^{\ell_1})$ has the dimensions $N \times N$ where N is the number of grid points. However, in general, the interpolation of a constant signal on a grid should also be a constant signal between the grid points and it is very natural to impose the normalization condition between the grid points as well:

$$\int H(\vec{x},\vec{y})\; d^3y \;=\sum_{\ell} h^{\ell}(\vec{x}) = 1\,. \tag{2.7}$$

The process of sampling a signal is very similar to a projection. However, the transformation (2.5) does not necessarily correspond to the application of a projective operator to $u_i(x)$. Indeed, if the signal is discrete-filtered again, the result is given by

$$\overline{\overline{u}}_i(\vec{x}) = \sum_{\ell_1}\; h^{\ell_1}(\vec{x})\;\sum_{\ell_2}\; h^{\ell_2}(\vec{x}^{\ell_1})\; u_i(\vec{x}^{\ell_2})\,, \tag{2.8}$$

and, introducing the N-dimensional vectors $u_i^{\ell_1} = u_i(x^{\ell_1})$, the discrete-filtering operator must satisfy the following constraint

$$\sum_{\ell_2}\; H^{\ell_1\ell_2}\; u_i^{\ell_2} = u_i^{\ell_1}\,, \tag{2.9}$$

in order to be considered as a projector. Remarkably enough, the same condition ensures that the discrete-filtered signal takes the same value as the Navier-Stokes signal on the grid points since the right-hand-side of relation (2.9) is simply $\overline{u}_i(\vec{x}^{\ell_2})$. The three vectors $u_i^{\ell_2}$ $(i = 1,2,3)$ are thus eigenvectors of the square matrix $H^{\ell_1\ell_2}$ with the eigenvalue $\lambda = 1$. These constraints, for three independent signals u_1, u_2 and u_3, are difficult to satisfy and, although no attempt will be done to prove it, the only solution seems to be:

$$H^{\ell_1\ell_2} = \delta^{\ell_1\ell_2}\,. \tag{2.10}$$

This choice automatically satisfies the normalization constraint as well.

It is also interesting that, imposing the projector constraint, the derivatives of these functions at the grid points entirely define the numerical scheme that has to be used when solving the discrete-filtered Navier-Stokes equations. Indeed, the derivatives of $\overline{u}_i$ on the grid are given by

$$\partial_m\overline{u}_i(\vec{x}^{\ell_1}) = \sum_{\ell_2}\; D_m^{\ell_1\ell_2}\; u_i(\vec{x}^{\ell_2}) = \sum_{\ell_2}\; D_m^{\ell_1\ell_2}\; \overline{u}_i(\vec{x}^{\ell_2})\,, \tag{2.11}$$

$$\partial^2_{mn}\overline{u}_i(\vec{x}^{\ell_1}) = \sum_{\ell_2}\; D_{mn}^{\ell_1\ell_2}\; u_i(\vec{x}^{\ell_2}) = \sum_{\ell_2}\; D_{mn}^{\ell_1\ell_2}\; \overline{u}_i(\vec{x}^{\ell_2})\,, \tag{2.12}$$

where the differentiation matrices are given by

$$D_m^{\ell_1\ell_2} = \frac{\partial h^{\ell_2}}{\partial x_m}(\vec{x}^{\ell_1})\,, \tag{2.13}$$

$$D_{mn}^{\ell_1\ell_2} = \frac{\partial^2 h^{\ell_2}}{\partial x_m \partial x_n}(\vec{x}^{\ell_1})\,. \tag{2.14}$$

The normalization constraint imposes:

$$\sum_{\ell_2} D_m^{\ell_1\ell_2} = 0\,, \tag{2.15}$$

$$\sum_{\ell_2} D_{mn}^{\ell_1\ell_2} = 0\,. \tag{2.16}$$

These constraints are fairly easy to satisfy.

3. Example

The simplest example of a finite difference scheme is probably the second order centered difference scheme on a regular one dimensional grid. In that case, the grid points are given by $x^\ell = L\,\ell/N$ where $\ell = 1\cdots N$. The signals will be assumed to be periodic and two grid points are added to the grid: $x^0 \equiv x^N$ and $x^{N+1} \equiv x^1$. The first and second derivatives of the discrete signal are given by:

$$\frac{\partial\overline{u}(x^\ell)}{\partial x} = \frac{\overline{u}(x^{\ell+1}) - \overline{u}(x^{\ell-1})}{2\Delta} \equiv \partial_x^\Delta \overline{u}\,, \tag{3.1}$$

$$\frac{\partial^2\overline{u}(x^\ell)}{\partial x^2} = \frac{\overline{u}(x^{\ell+1}) - 2\overline{u}(x^\ell) + \overline{u}(x^{\ell-1})}{\Delta^2} \equiv (\partial_x^\Delta)^2 \overline{u}\,, \tag{3.2}$$

where $\Delta = L/N$ is the grid spacing. The choice of function $h^\ell(x)$ is not unique, even when imposing (3.1) and (3.2). In order to simplify the structure of the function $h^\ell(x)$, only compact support functions will be considered. Moreover, since a homogeneous grid is assumed, it is reasonable to assume that the functions h^ℓ have all the same shape and are characterized by a single function:

$$h^\ell(x) = g\left(\frac{x - x^\ell}{\Delta}\right) \tag{3.3}$$

Since the constraints (3.1) and (3.2) only concern the first two neighbor points, the support will be assumed to be $[-3/2, 3/2]$ so that only three points are included in it. The connection points at $y = \pm 3/2$ might lead to discontinuities. However, as an additional constraint, the function g is assumed to be C^1. The second derivative is thus allowed to be discontinuous, but only between grid points. In that case, it is actually much easier to define $g(y)$ separately for three intervals as follows:

$$\begin{aligned} g(y) &= p_a(y)\ \Theta(\frac{1}{2} + y)\ \Theta(\frac{1}{2} - y) \\ &+ p_b(-y)\ \Theta(\frac{3}{2} + y)\ \Theta(-\frac{1}{2} - y) + p_b(y)\ \Theta(\frac{3}{2} - y)\ \Theta(-\frac{1}{2} + y)\,, \end{aligned} \tag{3.4}$$

where $\Theta(y)$ is the Heaviside function. This choice implies that $g(y) = g(-y)$, which is reasonable for a centered difference scheme. The constraint (2.10) imposes that $p_a(0) = 1$ and $p_b(1) = 0$. Taking into account (1) the fact that the functions h^ℓ are assumed to be all the same (3.3) and (2) the compact support of g, the normalization constraint reduces to $g(y) + g(y+1) + g(y-1) = 1$. Considering the structure (3.4), this imposes:

$$p_a(y) + p_b(y+1) + p_b(-y+1) = 1 \tag{3.5}$$

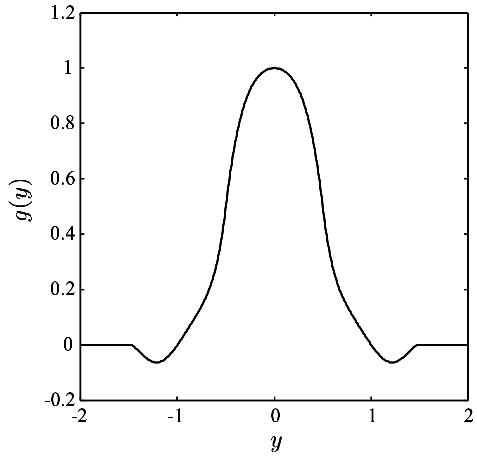

FIGURE 1. The function $g(y)$ defined by the expressions (3.4,3.6-3.7).

The lowest order polynomials that can be found to satisfy these constraints as well as the continuity of g and of its derivative at $y = \pm 3/2$ and $y = \pm 1/2$ are given by:

$$p_a(y) = 1 - y^2 - 4\,y^4\,, \tag{3.6}$$

$$p_b(y) = 2\,(1+y)\,(\frac{3}{2}+y)^2\,(2+5\,y+4\,y^2)\,. \tag{3.7}$$

The resulting function g is shown in the Figure 1. For summarizing the properties of the discrete-filtering operator, the above choice for the function g ensures that (on the grid):

$$\begin{aligned} \overline{u} &= u \\ \overline{u^2} &= \overline{u}^2\,, \\ \frac{\partial \overline{u}(x^\ell)}{\partial x} &= \frac{\overline{u}(x^{\ell+1}) - \overline{u}(x^{\ell-1})}{2\Delta} = \partial_x^\Delta \overline{u}(x^\ell)\,, \\ \frac{\partial^2 \overline{u}(x^\ell)}{\partial x^2} &= \frac{\overline{u}(x^{\ell+1}) - 2\overline{u}(x^\ell) + \overline{u}(x^{\ell-1})}{\Delta^2} = (\partial_x^\Delta)^2 \overline{u}(x^\ell)\,, \end{aligned}$$

and that (everywhere):

$$\overline{\overline{u}}(x) = \overline{u}(x)\,. \tag{3.8}$$

For three-dimensional systems, the function $h^\ell(\vec{x})$ is simply a product of one-dimensional functions g and the grid point coordinate x^ℓ can be characterized by a vector of indices (l_x, l_y, l_z):

$$h^{\{\ell_x,\ell_y,\ell_z\}}(\vec{x}) = g\left(\frac{x - x^{\ell_x}}{\Delta_x}\right)\; g\left(\frac{y - y^{\ell_y}}{\Delta_y}\right)\; g\left(\frac{z - z^{\ell_z}}{\Delta_z}\right)\,, \tag{3.9}$$

and $\vec{x}^\ell = (x^{\ell_x}, y^{\ell_y}, z^{\ell_z})$.

4. Interpolation and diagnostics

In the preceding sections, interpolation functions compatible with a given finite difference scheme have been introduced. They correspond to functions for which the derivatives on the grid are evaluated exactly by the spatial discretization scheme. The functions $h^{\ell_1}(\vec{x})$ thus play the same role for finite difference schemes as the plane waves $e^{i\vec{k}.\vec{x}}$ for

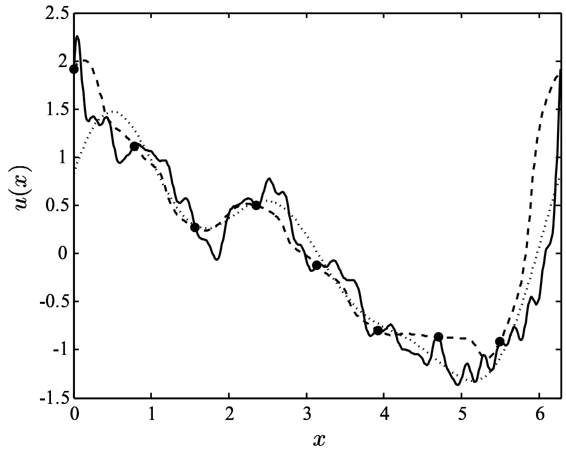

FIGURE 2. The comparison between the sampling operator and a sharp Fourier cutoff is shown for a one dimensional signal. The solid line corresponds to the original periodic signal on the interval $[0, 2\pi]$ built using 32 modes with random amplitudes. The dashed curve corresponds to the sampled signal on a 8 point grid reconstructed using the interpolation functions $h^\ell(x)$. The dotted line is obtained by applying a Fourier cutoff keeping 8 modes.

spectral methods. In that sense, their introduction improves the mathematical grounding of finite differences, though they do not modify the practical implementation of these numerical methods. The approach developed here could then be considered at first sight as an interesting mathematical framework for finite difference schemes but without practical implications. There are however practical implications. The first one is in the post-processing of results obtained using a finite difference scheme. Many quantities are routinely computed in a numerical simulation. It is not the purpose of this work to derive the influence of the interpolation function on the exhaustive list of possible diagnostics. Only two important quantities, the energy and the dissipation will be considered. Moreover, in order to simplify the discussion, the following developments are restricted to one-dimensional systems.

By definition, the one-dimensional kinetic energy is given by

$$E = \frac{1}{2} \int dx \; \overline{u}(x) \; \overline{u}(x) \,, \tag{4.1}$$

$$= \frac{1}{2} \sum_{\ell_1 \ell_2} \overline{u}(x^{\ell_1}) \; Q^{\ell_1 \ell_2} \; \overline{u}(x^{\ell_2}) \,, \tag{4.2}$$

where

$$Q^{\ell_1,\ell_2} = \int dx \; h^{\ell_1}(x) \; h^{\ell_2}(x) \,. \tag{4.3}$$

In spectral methods, thanks to the Parseval theorem, the matrix $Q^{\ell_1 \ell_2}$ reduces to δ^{ℓ_1,ℓ_2}. It is possible to impose this constraint for finite difference schemes at the expense of an increase in the degree of the polynomials used in the definition of the functions $h^{\ell_1}(\vec{x})$. However, the choice for the set of most relevant diagnostics is problem dependent. Any attempt to simplify their expression would thus make the definition of the function $h^\ell(\vec{x})$ problem dependent as well. To avoid this undesirable feature, the "simplest" functions $h^{\ell_1}(\vec{x})$ derived in the previous section and compatible with the continuity and normalization constraints as well as with the numerical scheme will be kept. Consequently, for the one dimensional second order centered finite difference scheme, the matrix $Q^{\ell_1 \ell_2}$ is not diagonal but can be evaluated explicitly:

$$Q^{\ell_1,\ell_2} = q_1\ \delta^{\ell_1,\ell_2} + q_2\ \left(\delta^{\ell_1,\ell_2+1} + \delta^{\ell_1,\ell_2-1}\right) + q_3\ \left(\delta^{\ell_1,\ell_2+2} + \delta^{\ell_1,\ell_2-2}\right)\ , \tag{4.4}$$

where $q_1 = 11339/13860$, $q_2 = 121/1260$ and $q_3 = -47/9240$. The property $q_1 + 2\,q_2 + 2\,q_3 = 1$ can be derived from the normalization properties of the functions $h^{\ell}(\vec{x})$.

Similarly, the one dimensional dissipation is defined by:

$$\mathcal{E} = 2\,\nu \int dx\ \left(\partial_x \overline{u}(x)\right)\ \left(\partial_x \overline{u}(x)\right)\ , \tag{4.5}$$

$$= 2\,\frac{\nu}{\Delta^2} \sum_{\ell_1 \ell_2} \overline{u}(x^{\ell_1})\ W^{\ell_1 \ell_2}\ \overline{u}(x^{\ell_2})\,, \tag{4.6}$$

where

$$W^{\ell_1,\ell_2} = \int d\vec{x}\ \left(\partial_x h^{\ell_1}(\vec{x})\right)\ \left(\partial_x h^{\ell_2}(\vec{x})\right)\ . \tag{4.7}$$

The matrix $W^{\ell_1 \ell_2}$ can also be evaluated and is given by:

$$W^{\ell_1,\ell_2} = w_1\ \delta^{\ell_1,\ell_2} + w_2\ \left(\delta^{\ell_1,\ell_2+1} + \delta^{\ell_1,\ell_2-1}\right) + w_3\ \left(\delta^{\ell_1,\ell_2+2} + \delta^{\ell_1,\ell_2-2}\right)\ , \tag{4.8}$$

where $w_1 = 1009/315$, $w_2 = -179/105$ and $w_3 = 13/126$. The property $w_1 + 2\,w_2 + 2\,w_3 = 0$ can also be derived from the normalization properties of the functions $h^{\ell}(\vec{x})$.

5. Dynamic Procedure

Another place where the sampling viewpoint has a direct influence is in the implementation of the dynamic procedure. Indeed, the definition of the velocity on the test-level grid requires the explicit definition of the coarsening operator.

There is no reason to expect the dynamic Smagorinsky model to be a good candidate for representing the effect of the commutation error between the discrete-filtering operator and the spatial derivative. However, since this model has been thoroughly benchmarked and, at the very least, has the property to be dissipative so that it should stabilize the simulation, there is some rationale to evaluate and test the dynamic procedure for this model as a first step.

Numerical simulations, both DNS and LES, can be seen as the time advancement of a discrete-filtered velocity. We will consider three grids: The DNS grid $\mathcal{G}^{\Delta_0}$, the LES grid $\mathcal{G}^{\Delta_1}$ and a test grid $\mathcal{G}^{\Delta_2}$ that is used only in the implementation of the dynamic procedure. In order to stress that the discrete-filtering operator is really based on the sampling concept, its application to the incompressible Navier-Stokes velocity is denoted by:

$$u_i^{\Delta_0} = \mathcal{S}^{\Delta_0} \circ u_i\,, \tag{5.1}$$

where $u_i^{\Delta_0}$ is the DNS field and the LES and test fields will be noted respectively $u_i^{\Delta_1}$ and $u_i^{\Delta_2}$. The three grids are assumed to be successively embedded $\mathcal{G}^{\Delta_2} \subset \mathcal{G}^{\Delta_1} \subset \mathcal{G}^{\Delta_0}$. This is enough to guarantee that

$$\mathcal{S}^{\Delta_2} = \mathcal{S}^{\Delta_2} \circ \mathcal{S}^{\Delta_1} = \mathcal{S}^{\Delta_2} \circ \mathcal{S}^{\Delta_1} \circ \mathcal{S}^{\Delta_0}\,, \tag{5.2}$$

$$\mathcal{S}^{\Delta_1} = \mathcal{S}^{\Delta_1} \circ \mathcal{S}^{\Delta_0}\,, \tag{5.3}$$

since only the grid point values of the velocity are used to construct the $u_i^{\Delta_0}$, $u_i^{\Delta_1}$ and

$u_i^{\triangle_2}$ velocities. The DNS equation can be written as:

$$\partial_t u_i^{\triangle_0} = \underbrace{-\partial_j^{\triangle_0} u_i^{\triangle_0} u_j^{\triangle_0} - \partial_i^{\triangle_0} p^{\triangle_0} + \nu \Delta^{\triangle_0} u_i^{\triangle_0}}_{N_i^{\triangle_0}(u^{\triangle_0})}, \tag{5.4}$$

where the differentiation operators $\partial_i^{\triangle_0}$ and $\Delta^{\triangle_0}$ define the numerical scheme used in the DNS. By definition, the discretization error and, in particular, the difference between the discrete-filtered value of the velocity derivative $(\partial_j u_i)^{\triangle_0}$ and its evaluation on the grid $\partial_j^{\triangle_0} u_i^{\triangle_0}$ is supposed to be small enough so that it need not be modelled. This is obviously not the case in the LES equation:

$$\partial_t u_i^{\triangle_1} = \underbrace{-\partial_j^{\triangle_1} u_i^{\triangle_1} u_j^{\triangle_1} - \partial_i^{\triangle_1} p^{\triangle_1} + \nu \Delta^{\triangle_1} u_i^{\triangle_1}}_{N_i^{\triangle_1}(u^{\triangle_1})} + \mathcal{E}_i^{\triangle_1,\triangle_0}, \tag{5.5}$$

and the additional term

$$\mathcal{E}_i^{\triangle_1,\triangle_0} = \mathcal{S}^{\triangle_1} \circ N_i^{\triangle_0}(u^{\triangle_0}) - N_i^{\triangle_1}(u^{\triangle_1}), \tag{5.6}$$

has to be modelled. It contains three contributions from the pressure, the convective and the viscous terms. Actually, these terms should be constructed using the Navier-Stokes equations instead of the DNS equations. However, since it is assumed that the DNS velocity is a fair representation of the actual velocity, the expression (5.6) is acceptable and allows a more homogeneous presentation. Using the same notations, the test-level equations can be written as

$$\partial_t u_i^{\triangle_2} = \underbrace{-\partial_j^{\triangle_2} u_i^{\triangle_2} u_j^{\triangle_2} - \partial_i^{\triangle_2} p^{\triangle_2} + \nu \Delta^{\triangle_2} u_i^{\triangle_2}}_{N_i^{\triangle_2}(u^{\triangle_2})} + \mathcal{E}_i^{\triangle_2,\triangle_0}, \tag{5.7}$$

and the additional term that has to be modelled at the test-level reads:

$$\mathcal{E}_i^{\triangle_2,\triangle_0} = \mathcal{S}^{\triangle_2} \circ N_i^{\triangle_0}(u^{\triangle_0}) - N_i^{\triangle_2}(u^{\triangle_2}). \tag{5.8}$$

Equivalently, the equations for $u_i^{\triangle_2}$ can be obtained by applying $\mathcal{S}^{\triangle_2}$ on the LES equations:

$$\partial_t u_i^{\triangle_2} = \mathcal{S}^{\triangle_2} \circ N_i^{\triangle_1}(u^{\triangle_1}) + \mathcal{S}^{\triangle_2} \circ \mathcal{E}_i^{\triangle_1,\triangle_0}, \tag{5.9}$$

Consistency between these two formulations imposes the following identity:

$$\mathcal{E}_i^{\triangle_2,\triangle_1} = \mathcal{E}_i^{\triangle_2,\triangle_0} - \mathcal{S}^{\triangle_2} \circ \mathcal{E}_i^{\triangle_1,\triangle_0}, \tag{5.10}$$

where

$$\mathcal{E}_i^{\triangle_2,\triangle_1} = \mathcal{S}^{\triangle_2} \circ N_i^{\triangle_1}(u^{\triangle_1}) - N_i^{\triangle_2}(u^{\triangle_2}). \tag{5.11}$$

Equation (5.10) is nothing else the equivalent of the Germano identity for discrete-filtering operators, written at the vector level instead of the tensor level. The term (5.11) is known in terms of the LES velocity only (since $u_i^{\triangle_2} = \mathcal{S}^{\triangle_2} \circ u_i^{\triangle_1}$) and plays the role of the Leonard tensor in the Germano identity. The right-hand-side depends on the terms that have to be modelled at both LES and test levels.

If the Smagorinsky model is used at both LES and test levels, the identity is only an approximation that reads:

$$\mathcal{E}_i^{\triangle_2,\triangle_1} \approx 2\ C\ M_i^{\triangle_2} \tag{5.12}$$

where

$$M_i^{\triangle_2} = \Delta_2^2\ \partial_j^{\triangle_2}\ |S^{\triangle_2}|\ S_{ij}^{\triangle_2} - \mathcal{S}^{\triangle_2} \circ \Delta_1^2\ \partial_j^{\triangle_1}\ |S^{\triangle_1}|\ S_{ij}^{\triangle_1}\,. \tag{5.13}$$

The tensor $S_{ij}^{\Delta_1}$ and $S_{ij}^{\Delta_2}$ represents the strain tensors evaluated on the LES and test grids respectively. The LES and test grid spacings are, respectively, Δ_1 and Δ_2. In this formulation, it is assumed that the Smagorinsky parameter C is constant in the entire volume and is the same at both LES and test levels. Its optimal value is given by:

$$C \approx \frac{1}{2} \frac{\langle \mathcal{E}_i^{\Delta_2,\Delta_1} M_i^{\Delta_2} \rangle}{\langle M_i^{\Delta_2} M_i^{\Delta_2} \rangle} . \tag{5.14}$$

Assuming that $\alpha = \Delta_2/\Delta_1$ is a constant, the dynamic procedure can be used to compute directly the constant $c = C\Delta_1^2$:

$$c \approx \frac{1}{2} \frac{\langle \mathcal{E}_i^{\Delta_2,\Delta_1} m_i^{\Delta_2} \rangle}{\langle m_i^{\Delta_2} m_i^{\Delta_2} \rangle} , \tag{5.15}$$

where

$$m_i^{\Delta_2} = \alpha^2 \ \partial_j^{\Delta_2} \ |S^{\Delta_2}| \ S_{ij}^{\Delta_2} - \mathcal{S}^{\Delta_2} \circ \partial_j^{\Delta_1} \ |S^{\Delta_1}| \ S_{ij}^{\Delta_1} , \tag{5.16}$$

and the model that has to be implemented in the code reads:

$$\mathcal{E}_i^{\Delta_1,\Delta_0} \approx 2 \ c \ \partial_j^{\Delta_1} \left(|S^{\Delta_1}| \ S_{ij}^{\Delta_1} \right) . \tag{5.17}$$

6. Numerical results

This model has been implemented in a pseudo-spectral code with modified wave vectors in order to mimic the behavior of a second-order centered finite difference scheme. Although this method is not computationally optimal, it has the advantage to be very easy to implement both for the DNS and for the LES. The computational domain is a cubic $2\pi \times 2\pi \times 2\pi$ box. The DNS grid, $\mathcal{G}^{\Delta_0}$, corresponds to a 256^3 resolution and the modified wave vectors for the finite difference scheme $\vec{\mathbf{k}}^{\mathrm{FD}}$ are defined by:

$$\vec{\mathbf{k}}^{\mathrm{FD}} = (k_x^{\mathrm{FD}}, k_y^{\mathrm{FD}}, k_y^{\mathrm{FD}}) = \frac{1}{\Delta_0} \left(\sin\left(k_x^{\mathrm{S}}\Delta_0\right), \sin\left(k_y^{\mathrm{S}}\Delta_0\right), \sin\left(k_z^{\mathrm{S}}\Delta_0\right)\right) , \tag{6.1}$$

$$(k^2)^{\mathrm{FD}} = \frac{4}{\Delta_0^2} \left(\sin^2\left(\frac{k_x^{\mathrm{S}}\Delta_0}{2}\right) + \sin^2\left(\frac{k_y^{\mathrm{S}}\Delta_0}{2}\right) + \sin^2\left(\frac{k_z^{\mathrm{S}}\Delta_0}{2}\right)\right) , \tag{6.2}$$

where $\vec{\mathbf{k}}^{\mathrm{S}}$ is the usual wave vector in the pseudo-spectral code. Note that, in the finite difference scheme, the discretization of the second order derivative is not obtained as the "square" of the first order derivative and consequently different definitions are used for the modified wave vectors entering the first and the second order derivatives. The quantity $(k^2)^{\mathrm{FD}}$ is only used in the viscous term. The incompressibility condition is enforced by projecting the velocity $\vec{u}(\vec{\mathbf{k}}^{\mathrm{FD}})$ on the plane perpendicular to $\vec{\mathbf{k}}^{\mathrm{FD}}$.

The sampling operators $\mathcal{S}^{\Delta_1}$ and $\mathcal{S}^{\Delta_2}$ are implemented straightforwardly in real space. It should be acknowledged however that enforcing incompressibility is an operation that now depends on the resolution. Consequently, it slightly modifies the properties of the sampling operators, and the velocity values on the grids $\mathcal{G}^{\Delta_0}$, $\mathcal{G}^{\Delta_1}$ and $\mathcal{G}^{\Delta_2}$ do not coincide exactly. The combination of the sampling and the incompressibility projections remains nevertheless a projective operator.

The LES field is thus obtained by sampling using $\mathcal{S}^{\Delta_1}$ on a 32^3 grid. The computations in the implementation of the dynamic procedure that corresponds to the grids $\mathcal{G}^{\Delta_1}$ and $\mathcal{G}^{\Delta_2}$ are then performed by a simple re-definition of the modified wave vectors.

The preliminary tests, though made with a modified spectral code and a limited resolution, are quite illuminating. First, it shows clearly that a model is required for the

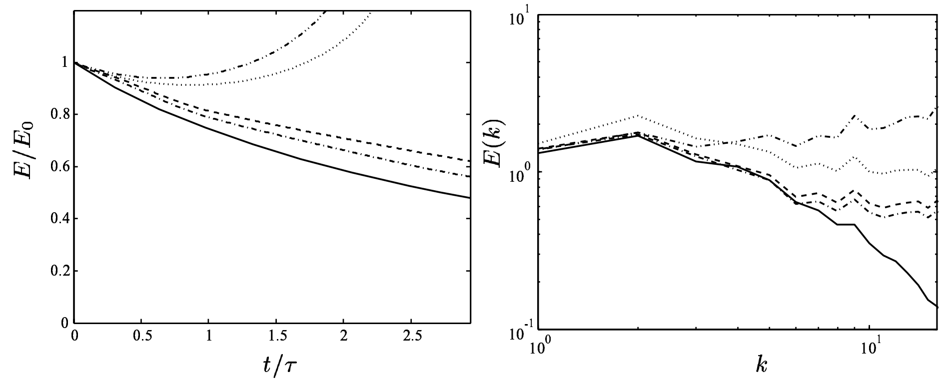

FIGURE 3. Left : Energy decay. Comparison between the sampled DNS (———), the LES curves without model (········) and with the dynamic Smagorinsky model with the parameter C computed using both convective and viscous contributions (– – – –), the convective contribution only (–·–·–) and the viscous contribution only (–··–··). Right : Energy spectrum at the end of the computation, same symbols. τ is the large-eddy turnover time.

decaying turbulence case. The under-resolved DNS (LES without model) exhibits an increase of the energy after a short decaying period. The dynamic Smagorinsky model has been implemented in three versions. Indeed, the "Leonard" vector $\mathcal{E}_i^{\Delta_2,\Delta_1}$ (5.11) contains two contributions originating respectively from the convective+pressure terms and from the viscous term. In the computation of the dynamic Smagorinsky constant C, the purely convective, the purely viscous, and the full Leonard vectors have been implemented. Not surprisingly, the purely viscous version does not perform satisfactorily. It is actually even worse that the no-model case. Also, the purely convective version produces the best agreement with the sampled DNS. The final spectra are also presented. They all exhibit a piling-up of the energy in the high wave-number range. However, the no-model and the purely viscous dynamic model both overpredict the low wave-number energy range, while the dynamic models that account for the convective discretization errors both correctly predict the low k spectrum.

Although it would be quite hazardous to make definitive and strong statements on the basis of these preliminary numerical results, they indicate that (1) the implementation of a dynamic procedure with sampling operators yields reasonable predictions in the homogeneous decaying turbulence test case and (2) the Smagorinsky model is acceptable for modelling the numerical discretization errors on the convective term but not for the viscous term.

7. Discussion

The methodology presented here is unusual in the sense that no filter is used to define the LES fields. The unknown quantities that appear in the LES equations thus originate only from the lack of resolution (discretization errors) and filters are replaced by sampling operators. The resulting viewpoint seems to make the link between finite difference approaches and finite element methods. The sampling operators have some very pleasant properties. They commute with nonlinearities, they are projections and they explicitly define the numerical grid. The obvious drawback is that they do not commute with spatial derivatives and the commutation errors must be modelled. It has been shown that models for the discretization errors may be treated using the dynamic procedure. Preliminary results, using the Smagorinsky model, are very encouraging, though the modelling of discretization errors by an eddy viscosity term may be debatable.

Considering the encouraging numerical results obtained in the very simple tests presented in section VI, it can be concluded that the methodology in which a LES is defined by sampling operators deserves, at the very least, further investigations. It is however not the purpose of this last section to oversell the sampling-based LES approach. We have thus chosen to close this discussion by pointing out two difficulties that have been raised in the course of the Summer Program and that definitively deserve some attention.

First, as mentioned before, the sampling operators do not preserve the incompressibility of the flow. This difficulty has to be expected since the incompressibility condition involves spatial derivatives:

$$\partial_i u_i = 0\,. \tag{7.1}$$

The non-commutation of the sampling operator and the spatial derivative thus generates an unknown term in the sampled version of Eq. (7.1). This unknown term has been neglected in the preliminary tests presented here. The modelling of such a term would probably be fairly difficult and might change the nature of the numerical scheme itself since the incompressibility condition is a very strong constraint in most numerical methods. To the best of our knowledge, the commutation error in the incompressibility condition has never been taken into account in more traditional LES in which non-commutative filters are also used. It might turn out that the only practical strategy is to ignore this effect, but numerical and theoretical investigations of the commutation error in the incompressibility condition would be welcome.

The second difficulty has been pointed out by O. Vasilyev: the sampling operators do not conserve the mean of the original signal. This can easily be seen if a sine wave with zero mean is sampled systematically at the minima, the resulting sampled signal would be constant and negative. This is a special case of aliasing due to too coarse sampling. Whether this is an important issue or not is not yet clear. Obviously, it has no damaging consequences in the isotropic turbulence tests. However, the consequences in complex geometries with mean flows remain to be explored.

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